

Solution 1: Entropy

A fair die is rolled at the same time as a fair coin is tossed. Let A be the number on the upper surface of the die and let B describe the outcome of the coin toss, where

$$B = \begin{cases} 1, & \text{head,} \\ 0, & \text{tail.} \end{cases}$$

Two random variables X and Y are given by $X = A + B$ and $Y = A - B$, respectively.

- (a) Calculate the entropies $H(X)$ and $H(Y)$, the conditional entropies $H(Y|X)$ and $H(X|Y)$, the joint entropy $H(X, Y)$ and the mutual information $I(X; Y)$.

Solution:

Let a, b, x , and y denote the realisations of the random variables A, B, X , and Y , respectively. Each event (a, b) is associated with exactly one event (x, y) and the probability for such an event is given by

$$p_{AB}(a, b) = p_{XY}(x, y) = \frac{1}{6} \cdot \frac{1}{2} = \frac{1}{12}$$

Consequently, we obtain for the joint entropy

$$\begin{aligned} H(X, Y) &= - \sum_{x, y} p_{X, Y}(x, y) \log_2 p_{X, Y}(x, y) = -12 \cdot \frac{1}{12} \log_2 \frac{1}{12} \\ &= \log_2 12 \\ &= 2 + \log_2 3 \end{aligned}$$

Below we list the possible values of the random variables X and Y , the associated events (a, b) , and the probability masses $p_X(x)$ and $p_Y(y)$.

x	events (a, b)	$p_X(x)$	y	events (a, b)	$p_Y(y)$
1	(1, 0)	1/12	0	(1, 1)	1/12
2	(2, 0), (1, 1)	1/6	1	(1, 0), (2, 1)	1/6
3	(3, 0), (2, 1)	1/6	2	(2, 0), (3, 1)	1/6
4	(4, 0), (3, 1)	1/6	3	(3, 0), (4, 1)	1/6
5	(5, 0), (4, 1)	1/6	4	(4, 0), (5, 1)	1/6
6	(6, 0), (5, 1)	1/6	5	(5, 0), (6, 1)	1/6
7	(6, 1)	1/12	6	(6, 0)	1/12

The random variable $X = A + B$ can take the values 1 to 7. The probability masses $p_X(x)$ for the values 1 and 7 are equal to 1/12, since they correspond to exactly one event. The probability masses for the values 2 to 6 are equal to 1/6, since each of these values corresponds to two events (a, b) . An analogue result is obtained for the random variable $Y = A - B$.

The marginal entropies are given by

$$\begin{aligned} H(X) &= - \sum_x p_X(x) \log_2 p_X(x) \\ &= -2 \cdot \frac{1}{12} \log_2 \frac{1}{12} - 5 \cdot \frac{1}{6} \log_2 \frac{1}{6} \\ &= \frac{1}{6} \cdot (\log_2 4 + \log_2 3) + \frac{5}{6} \cdot (\log_2 2 + \log_2 3) \\ &= \frac{7}{6} + \log_2 3 \end{aligned}$$

and for Y

$$\begin{aligned}
 H(Y) &= - \sum_y p_Y(y) \log_2 p_Y(y) \\
 &= -2 \cdot \frac{1}{12} \log_2 \frac{1}{12} - 5 \cdot \frac{1}{6} \log_2 \frac{1}{6} \\
 &= \frac{1}{6} \cdot (\log_2 4 + \log_2 3) + \frac{5}{6} \cdot (\log_2 2 + \log_2 3) \\
 &= \frac{7}{6} + \log_2 3
 \end{aligned}$$

We can determine the conditional entropies using

$$H(X|Y) = H(X, Y) - H(Y) = 2 + \log_2 3 - \frac{7}{6} - \log_2 3 = \frac{5}{6}$$

$$H(Y|X) = H(X, Y) - H(X) = 2 + \log_2 3 - \frac{7}{6} - \log_2 3 = \frac{5}{6}$$

The mutual information $I(X; Y)$ can be determined according to

$$I(X; Y) = H(X) - H(X|Y) = \frac{7}{6} + \log_2 3 - \frac{5}{6} = \frac{1}{3} + \log_2 3$$

or

$$I(X; Y) = H(Y) - H(Y|X) = \frac{7}{6} + \log_2 3 - \frac{5}{6} = \frac{1}{3} + \log_2 3$$

(b) Show that, for independent discrete random variables X and Y ,

$$I(X; X + Y) - I(Y; X + Y) = H(X) - H(Y)$$

Solution:

Using the definition of mutual information for discrete random variables, $I(X; Y) = H(Y) - H(Y|X)$, we can write

$$\begin{aligned}
 I(X; X + Y) - I(Y; X + Y) &= H(X + Y) - H(X + Y|X) - H(X + Y) + H(X + Y|Y) \\
 &= H(X|Y) - H(Y|X) \\
 &= H(X) - H(Y).
 \end{aligned}$$

The first step follows from the fact that modifying the mean of a pmf doesn't change the entropy. For the second step, we used the fact that the conditional entropy $H(X|Y)$ is equal to the marginal entropy $H(X)$ for independent random variables X and Y .

Solution 2: The Mutual Information of Three Variables

(a) According to the definition of mutual information, we have

$$\begin{aligned}
 &I(X; Y) - I(X; Y|Z) \\
 &= \sum_x \sum_y p(x, y) \log \frac{p(x, y)}{p(x)p(y)} - \underbrace{\sum_z \sum_x \sum_y p(z)p(x, y|z) \log \frac{p(x, y|z)}{p(x|z)p(y|z)}}_{\text{The definition of conditional mutual information}} \\
 &= \sum_x \sum_y \sum_z p(x, y, z) \log \frac{p(x, y)}{p(x)p(y)} - \sum_x \sum_y \sum_z p(x, y, z) \log \frac{p(x, y|z)p(z)^2}{p(x|z)p(y|z)p(z)^2} \\
 &= \sum_x \sum_y \sum_z p(x, y, z) \log \frac{p(x, y)}{p(x)p(y)} - \sum_x \sum_y \sum_z p(x, y, z) \log \frac{p(x, y, z)p(z)}{p(x, z)p(y, z)} \\
 &= \sum_x \sum_y \sum_z p(x, y, z) \log \left(\frac{p(x, y)p(x, z)p(y, z)}{p(x)p(y)p(z)p(x, y, z)} \right) \\
 &= I(X; Y; Z).
 \end{aligned} \tag{1}$$

(b) Using the lemma we just proved, we obtain:

$$\begin{aligned}
 & I(X; Y|Z) + I(Y; Z) - I(Y; Z|X) \\
 &= I(X; Y) - I(X; Y; Z) + I(Y; Z) - I(Y; Z) + I(X; Y; Z) \\
 &= I(X; Y).
 \end{aligned} \tag{2}$$

(P.S., a recent paper [1] provides a good example of how this relation is used in the research of explainability.)

Solution 3: Smoothed Cross-Entropy Loss

(a) The empirical risk is

$$\begin{aligned}
 R_{\text{emp}} &= \frac{1}{n} \sum_{i=1}^n \left(\sum_{k=1}^g \tilde{d}_k^{(i)} \log \left(\frac{\tilde{d}_k^{(i)}}{\pi_k(\mathbf{x}^{(i)}|\theta)} \right) \right) \\
 &= \frac{1}{n} \sum_{i=1}^n \left(\sum_{k=1}^g \tilde{d}_k^{(i)} \log \tilde{d}_k^{(i)} - \tilde{d}_k^{(i)} \log \pi_k(\mathbf{x}^{(i)}|\theta) \right) \\
 &= -\frac{1}{n} \sum_{i=1}^n \sum_{k=1}^g \tilde{d}_k^{(i)} \log \pi_k(\mathbf{x}^{(i)}|\theta) + \text{Const.}
 \end{aligned} \tag{3}$$

(b) The smoothed cross-entropy is implemented as follows:

```

#' @param label ground truth vector of the form (n_samples,).
#' Labels should be "1","2","3" and so on.
#' @param pred Predicted probabilities of the form (n_samples,n_labels)
#' @param smoothing Hyperparameter for label-smoothing

smoothed_ce_loss <- function(
  label,
  pred,
  smoothing){

  num_samples <- NROW(pred)
  num_classes<- NCOL(pred)

  # Let's make some assertions:
  # label should be a 1-D array.one-hot encoded label is not necessary
  stopifnot(NCOL(label)==1)
  # smoothing hyperparameter in allowed range
  stopifnot((smoothing>=0 & smoothing <= 1))
  # Same amount of rows in labels and predictions
  stopifnot((NROW(label)== num_samples))
  # Predicted probabilities must have as many columns as labels
  stopifnot(length(unique(label)) == num_classes)

  #Calculate the base level
  smoothing_per_class <- smoothing / num_classes

  # build the label matrix. Shape = [ num_samples, num_classes]
  # Start with the base level
  smoothed_labels_matrix = matrix(smoothing_per_class,
                                   nrow=num_samples,ncol=num_classes)

  # Add the smoothed correct labels
  true_labels_loc=cbind(1:num_samples, label)
  smoothed_labels_matrix[true_labels_loc]= 1 - smoothing + smoothing_per_class
  cat("Labels matrix:\n")
  print(smoothed_labels_matrix)
}

```

```

# Calculate the loss
cat("Loss for each sample:\n ",
    rowSums(- smoothed_labels_matrix * log(pred)))

loss <- mean(rowSums(- smoothed_labels_matrix * log(pred)))
cat("\n Loss:\n",loss)

return (loss)
}

```

```

# Let's build a "confident model", the model has very high predicted
#probabilities for one of the labels
label= c(1,2,2,3,1)
pred= rbind(
    c(0.85,0.10,0.05),
    c(0.05,0.9,0.05),
    c(0.02,0.95,0.03),
    c(0.13,0.02,0.85),
    c(0.86,0.04,0.1))

# cross entropy means smoothing=0
smoothing=0
loss<-smoothed_ce_loss(label,pred,smoothing)

## Labels matrix:
##      [,1] [,2] [,3]
## [1,]    1    0    0
## [2,]    0    1    0
## [3,]    0    1    0
## [4,]    0    0    1
## [5,]    1    0    0
## Loss for each sample:
##    0.1625189 0.1053605 0.05129329 0.1625189 0.1508229
## Loss:
##    0.1265029

# Smoothed cross entropy
smoothing=0.2
loss_smooth<-smoothed_ce_loss(label,pred,smoothing)

## Labels matrix:
##      [,1]      [,2]      [,3]
## [1,] 0.86666667 0.06666667 0.06666667
## [2,] 0.06666667 0.86666667 0.06666667
## [3,] 0.06666667 0.86666667 0.06666667
## [4,] 0.06666667 0.06666667 0.86666667
## [5,] 0.86666667 0.06666667 0.06666667
## Loss for each sample:
##    0.4940709 0.4907434 0.5390262 0.537666 0.4988106
## Loss:
##    0.5120634

```

References

- [1] Rong, Yao, Tobias Leemann, Vadim Borisov, Gjergji Kasneci, and Enkelejda Kasneci. "A consistent and efficient evaluation strategy for attribution methods." In International Conference on Machine Learning, pp. 18770-18795.

